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# Introduction to NEAMS Fuel Modeling

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# Objective of the Fuels Product Line

- **The objective of the Fuels Product Line is to develop and deliver a mechanistic (i.e., predictive) computational toolset for nuclear fuel design and/or analysis**
  - Near-term Emphasis: oxide fuels for LWR applications; irradiation performance in quasi-steady state, operational transients, accident scenarios; integration/coupling with toolset being developed by the Reactors Product Line (via the NEAMS Workbench)
  - Longer-term Plans: additional fuel compositions/forms and reactor applications

- **Potential Applications**
  - Current & Future LWRs: better informed safety margins and operational constraints, power up-rates, burnup extension, spent fuel storage, accident-tolerant fuel analyses
  - Advanced Fuels: accelerated design and qualification of new fuels

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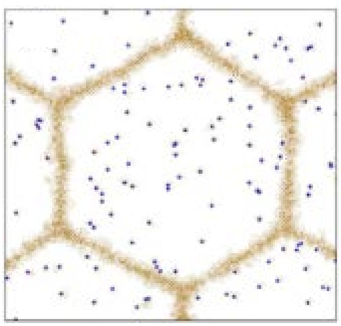
# Multiscale Modeling Approach to Achieve Genuine Predictability

- **Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds**
- **Goal: Develop improved, mechanistic, and predictive models for fuel performance using hierarchical, multiscale modeling**

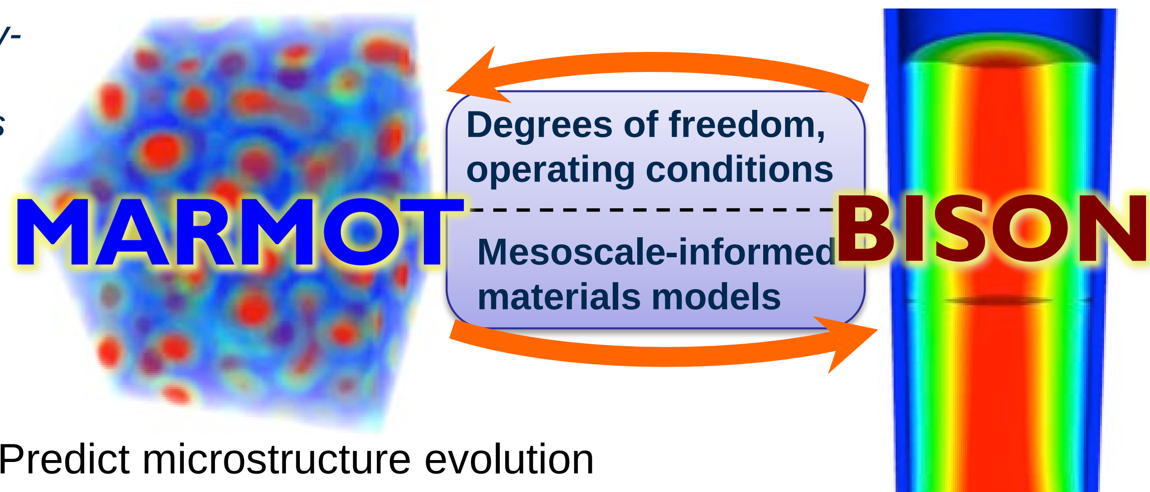
**Atomistic simulations**



*Atomistically-informed parameters*

**Meso-scale models**

**Fuel performance models**




- Identify important mechanisms
- Determine material parameter values

- Predict microstructure evolution
- Determine effect of evolution on material properties

- Predict fuel performance and failure probability

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# Multiscale Modeling Approach to Achieve Genuine Predictability

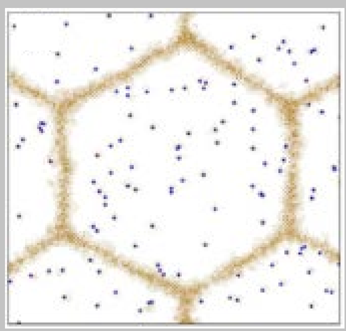
- Empirical models can accurately interpolate between data, but cannot ...polate outside of test bounds
- ...improv... ...redictive...
- ...ing hie... ...odeling

**Atomistic Modeling Methods**
David Andersson

**MARMOT Overview**
Yongfeng Zhang

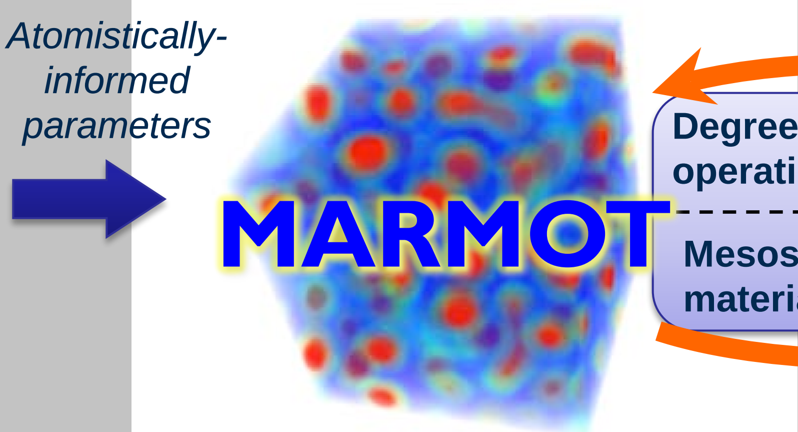
**BISON Overview**
Jason Hales

**Atomistic simulations**



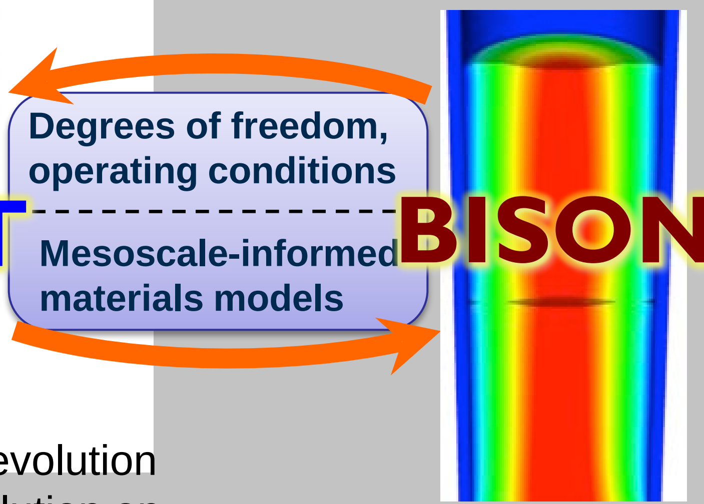
- Identify important mechanisms
- Determine material parameter values

**Meso-scale models**




- Predict microstructure evolution
- Determine effect of evolution on material properties

**Fuel performance models**




- Predict fuel performance and failure probability

# Thank You

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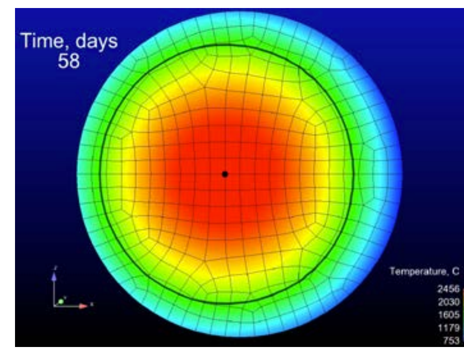
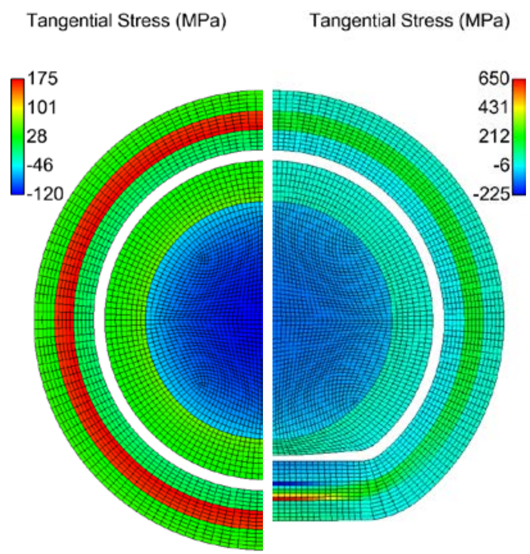
# BISON Update & Release

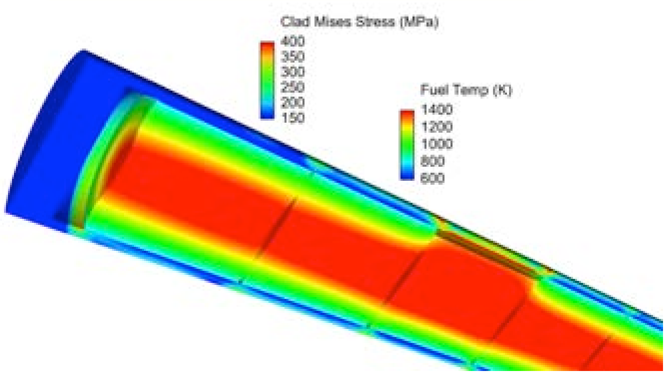
BISON 1.3

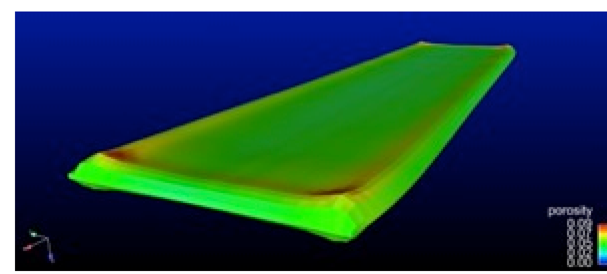
- **Update/release of BISON** (09/30/16)
  - Enhanced, mature, increasingly comprehensive capability to simulate oxide fuels for LWRs under quasi-steady state and off-normal conditions
  - Developing capabilities to model:
    - TRISO fuels for gas-cooled reactors, LWRs, FHRs
    - Metallic and oxide fuels for fast reactors
    - Plate-type fuels for research reactors




Annual Updates:
1) **User Manual**
2) **Theory Manual**
3) **Assessment Report**




BISON

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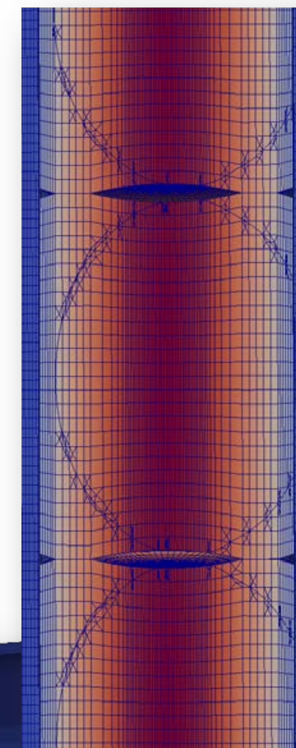
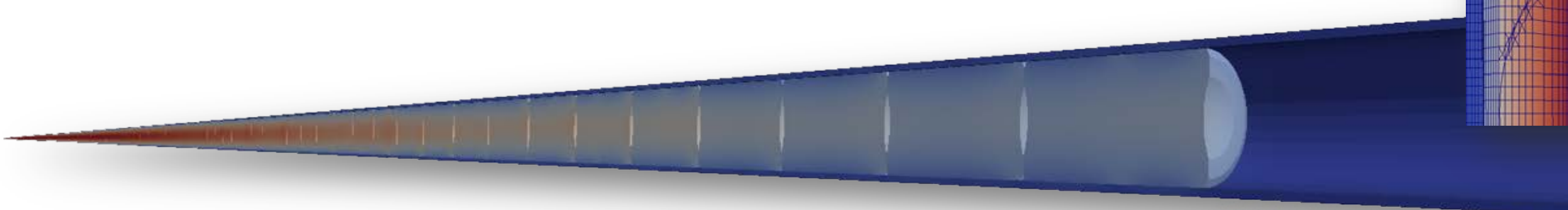
# Engineering-scale Tool Development

- **Development/validation of tools for predicting fuel performance at the engineering scale** (e.g., pellet-resolved fuel pins)
  - Applicable to normal, off-normal, accident conditions
  - Make use of advanced computational methods
    - High fidelity geometric representations
    - Highly efficient solvers to enable fully-coupled, multiphysics simulations
  - Required interfaces
    - Interface/couple with meso-scale tools developed by **FPL**
    - Interface/couple with assembly-scale tools developed by **RPL**
    - Executable on desktop workstations and high performance supercomputers
  - Phased development approach
    1) Make immediate use of existing (largely empirical) models for material properties/fuel behavior, recognizing limits of applicability
    2) Incorporate results from **Lower Length-scale Model Development** to enhance predictive power





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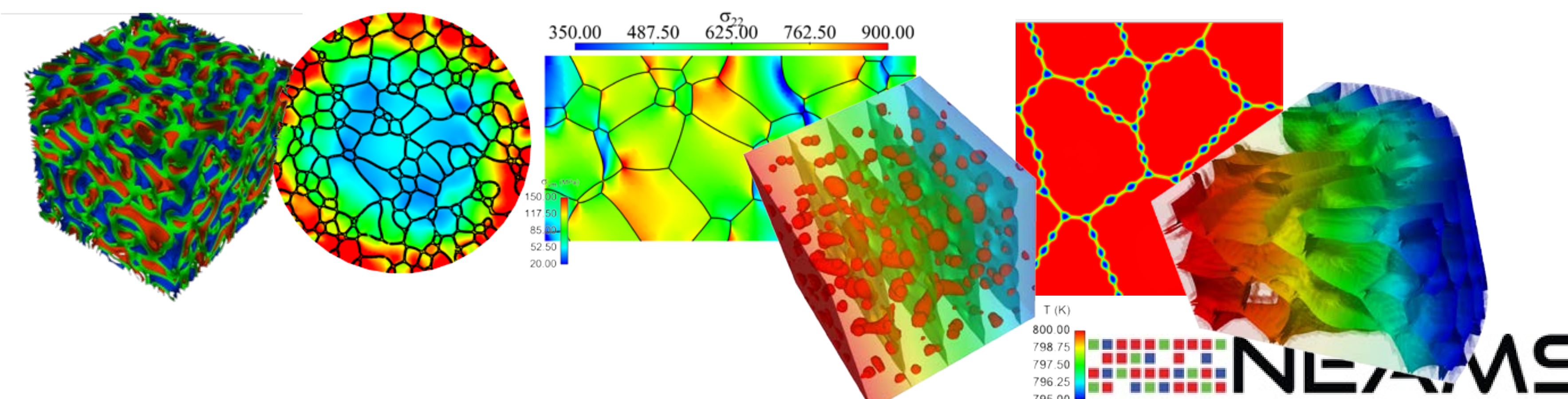
# Lower Length-scale Model Development

- **Development/validation of tools for simulating meso-scale, microstructure evolution under irradiation**
  - Atomic-scale simulations to enable meso-scale modeling
  - Tools to be used to
    - Develop fundamental material property/fuel behavior models
    - Up-scale to inform fuel performance simulations at engineering-scale
  - Reduce dependence on empirical correlations/models
  - Enable true predictability in compositional or operational regimes where little or no experimental data exists.

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